Gas phase enthalpies of formation for potential nitro-substituted borazine high energy materials: A G4MP2 and G4 theoretical study

Sierra Rayne [a] *, Kaya Forest [b]

Keywords: nitro-substituted borazines, high energy materials, enthalpy of formation, Gaussian-4 (G4), G4MP2, theoretical study

Gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_f H^\circ_{(g)}$) were calculated at the G4MP2 and G4 levels of theory using the atomization energy approach for various nitro-substituted borazines proposed as high energy materials (HEMs). Modest general agreement was obtained between the G4MP2/G4 atomization energy $\Delta_f H^\circ_{(g)}$ estimates and those previously reported using density functional theory methods and homodesmic reaction approaches, with deviations ranging between +9.7 to -56.5 kJ/mol. The results should help constrain the actual enthalpies of formation for these potential HEMs, and suggest the nitroborazines are a particularly challenging case for $\Delta_f H^\circ_{(g)}$ calculations using theoretical approaches, requiring high-level composite methods to obtain reliable $\Delta_f H^\circ_{(g)}$ estimates.

Nitroborazines have been proposed as potential high energy materials (HEMs) [1] (Figure 1). Their gas phase enthalpies of formation ($\Delta_f H^\circ_{(g)}$) have not been experimentally determined, but previous theoretical estimates have been put forward in the literature at the B3LYP/6-311+G(d,p) level of theory (Table 1). In the current work, we employ the G4MP2 [2] and G4 [3] composite method levels of theory within Gaussian 09 (G09) [4] and apply the atomization energy approach in ref. [5, 6] to provide additional $\Delta_f H^\circ_{(g)}$ estimates at 298.15 K and 1 atm for these compounds. Singlet and triplet calculations were performed on all compounds; no triplet ground states were observed. G09 archive entries are provided in the Supplementary Materials for all compounds.

Modest general agreement was obtained between our G4MP2 and G4 atomization energy $\Delta_f H^\circ_{(g)}$ estimates for **1** to **8** and those previously reported using density functional theory methods and homodesmic reaction $\Delta_f H^\circ_{(g)}$ approaches. Deviations between our G4MP2 $\Delta_f H^\circ_{(g)}$ estimates and the B3LYP/6-311+G(d,p) data by Janning and Ball [1] range from +9.7 to -56.5 kJ/mol, with the absolute deviation increasing with increasing molecular mass (generally related to increasing nitro-substitution). For B- and N-nitroborazine, G4 calculations obtained $\Delta_f H^\circ_{(g)}$ that were 21.0 and 16.6 kJ/mol lower than the DFT estimates, and 25.2 and 26.3 kJ/mol lower than the G4MP2 estimates, respectively. G4 calculations were not completed on **3** to **8** due to the computational costs.

Because of the large theory level differences in estimated $\Delta_f H^\circ_{(g)}$ for these potential HEMs, we also sought to validate the G4MP2 atomization energy approach for 15 borane derivatives with available experimental $\Delta_f H^\circ_{(g)}$ data (Table 2). We obtained good agreement between the experimental and predicted $\Delta_f H^\circ_{(g)}$ with no evidence of molecular size scaling errors, yielding mean unsigned, mean signed, and root mean squared deviations of 4.8, 7.0, and 10.1 kJ/mol, respectively, between the G4MP2 and experimental $\Delta_f H^\circ_{(g)}$ data. Similarly, a G4 $\Delta_f H^\circ_{(g)}$ estimate for borazine gave a value of -504.5 kJ/mol, in better agreement with the experimental value of -510.0 kJ/mol [8] than the G4MP2 estimate of -484.6 kJ/mol. Consequently, assuming that the G4 level of theory also provides atomization energy method $\Delta_f H^\circ_{(g)}$ estimates for substituted borazines with effective chemical accuracy, the G4MP2 $\Delta_f H^\circ_{(g)}$ results provided herein are likely overestimated by about 20 to 25 kJ/mol compared to their actual values. Overall, the results suggest the nitroborazines are a particularly challenging

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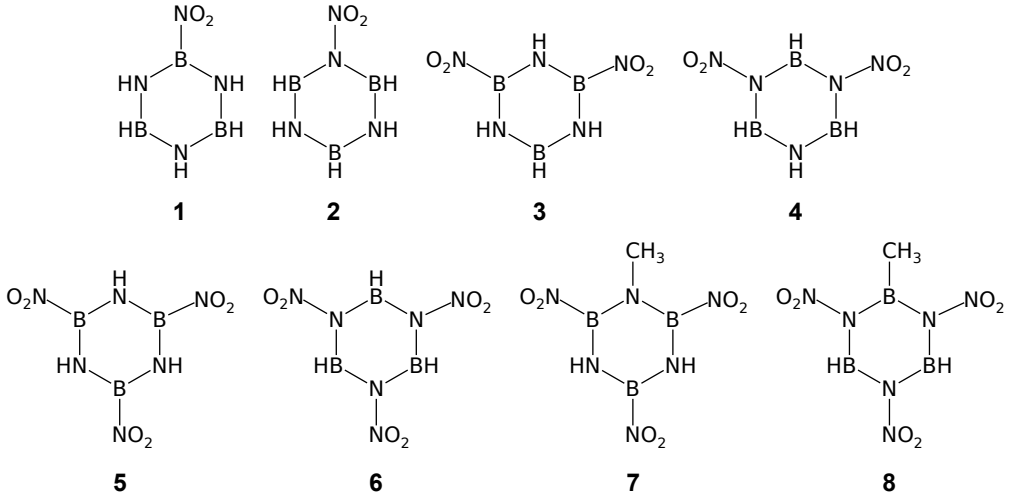

Figure 1: Structures of the nitro-substituted borazines under study.

Table 1: Estimated gas phase enthalpies of formation ($\Delta_f H^\circ_{(g)}$) at 298.15 K and 1 atm for various nitro-substituted borazines at the B3LYP/6-311+G(d,p) [1], G4MP2, and G4 levels of theory. Values are in kJ/mol.

compound	B3LYP/6-311+G(d,p) [1]	G4MP2	G4
B-nitroborazine (**1**)	-593.5	-589.3	-614.5
N-nitroborazine (**2**)	-418.6	-408.9	-435.2
B-dinitroborazine (**3**)	-677.1	-681.9	n/a[a]
N-dinitroborazine (**4**)	-326.4	-320.7	n/a
B-trinitroborazine (**5**)	-720.5	-763.7	n/a
N-trinitroborazine (**6**)	-195.5	-222.5	n/a
methyl-B-trinitroborazine (**7**)	-680.3	-736.8	n/a
methyl-N-trinitroborazine (**8**)	-245.7	-288.5	n/a

[a] not completed due to computational expense.

Table 2: Comparison between G4MP2 estimated gas phase enthalpies of formation ($\Delta_f H^\circ_{(g)}$) at 298.15 K and 1 atm for various borane derivatives with corresponding experimental data. Values are in kJ/mol.

compound	G4MP2	expt. [7]
BH_3	104.4	106.7 [8]
$B(OH)_3$	-994.7	-992.3 [8]
BF_2H	-730.5	-733.9 [8]
BF_3	-1130.1	-1135.6±0.8 [9], -1136.0 [8]
$BClF_2$	-885.3	-885.3 [8]
BCl_2H	-252.5	-248.1 [8]
BCl_2F	-644.1	-644.3 [8]
BCl_3	-409.8	-403.0 [8]
$BBrF_2$	-809.5	-820.1 [8]
$BBrCl_2$	-336.3	-336.8 [8]
BBr_2H	-105.4	-104.6 [8]
BBr_2F	-494.6	-514.6 [8]
BBr_2Cl	-263.2	-272.0 [8]
BBr_3	-190.7	-204.2 [8]
borazine	-484.6	-510.0 [8]

case for $\Delta_f H^\circ_{(g)}$ calculations using theoretical methods, and that the highest level composite (e.g., Gn and Wn) approaches currently available are necessary to obtain reliable $\Delta_f H^\circ_{(g)}$ estimates.

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References

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Supplementary Material: Gas phase enthalpies of formation for potential nitro-substituted borazine high energy materials: A G4MP2 and G4 theoretical study.

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G4MP2 archive entries

B-nitroborazine

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Temperature=              298.150000 Pressure=                    1.000000
E(ZPE)=                     0.096001 E(Thermal)=                  0.103860
E(CCSD(T))=              -445.974395 E(Empiric)=                 -0.217856
DE(MP2)=                   -0.507320 DE(HF)=                     -0.043613
G4MP2(0 K)=              -446.647182 G4MP2 Energy=             -446.639323
G4MP2 Enthalpy=          -446.638379 G4MP2 Free Energy=        -446.680076
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N-nitroborazine

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E(CCSD(T))=               -445.908411 E(Empiric)=                  -0.217856
DE(MP2)=                    -0.502183 DE(HF)=                      -0.044125
G4MP2(0 K)=               -446.578356 G4MP2 Energy=              -446.570619
G4MP2 Enthalpy=           -446.569675 G4MP2 Free Energy=         -446.611149
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DE(MP2)=                   -0.723900 DE(HF)=                      -0.064088
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G4MP2 Enthalpy=          -650.991070 G4MP2 Free Energy=         -651.040205
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G4MP2 Enthalpy=           -650.853480 G4MP2 Free Energy=         -650.902143
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B-trinitroborazine

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DE(MP2)=                   -0.940504 DE(HF)=                      -0.084521
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G4MP2 Enthalpy=          -855.339601 G4MP2 Free Energy=         -855.396287
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as2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-851.9545493\MP2/GTMP2LargeXP=-85
4.9068261\HF/GFHFB3=-851.963679\HF/GFHFB4=-852.0242992\G4MP2=-855.3539
669\FreqCoord=0.0018226181,0.0079272186,0.0093589548,2.66638477,0.0634
044333,0.020995155,3.9318650387,2.4088544198,-0.0005247886,2.551754870
2,4.688573419,-0.0335423011,-0.1123061864,4.6113627481,-0.0449947935,-
1.3971323489,2.2762948029,-0.023648257,-1.6304241889,7.0992723779,-0.0
81133295,-3.9483374665,6.9420679752,-0.090033265,-0.4296846967,9.08817
19327,-0.0988057039,6.8454670746,2.4811263356,0.0121423942,7.866895846
3,4.5676517307,-0.0074665879,7.9688406971,0.4477652619,0.0411141839,-1
.3912326392,-2.5522156439,0.0329290843,-3.7140652669,-2.5102111499,0.0
21186823,-0.0935192204,-4.4790611592,0.0620450074,3.6641628719,-1.5699
738827,0.0446635592,3.4669506528,6.3697174338,-0.0489109301,-3.3107025
153,2.2286993741,-0.0319378546\PG=C01 [X(B3H3N6O6)]\NImag=0\\
```

N-trinitroborazine

```
Temperature=               298.150000 Pressure=                     1.000000
E(ZPE)=                      0.096981 E(Thermal)=                   0.110059
E(CCSD(T))=               -853.862195 E(Empiric)=                  -0.369408
DE(MP2)=                    -0.926916 DE(HF)=                      -0.085951
G4MP2(0 K)=               -855.147489 G4MP2 Energy=              -855.134412
G4MP2 Enthalpy=           -855.133468 G4MP2 Free Energy=         -855.189404
1\1\GINC-CL1N142\Mixed\G4MP2\G4MP2\B3H3N6O6\KFOREST\13-Jan-2011\0\\# G
4MP2\\<< job name >>\\0,1\N,0,0.0238542178,0.0432641961,-0.0062926336\
B,0,1.4621156379,0.0058490965,0.0119447594\N,0,2.0922520619,1.29958700
61,-0.0029696677\B,0,1.4052948649,2.5640086775,-0.0229852032\N,0,-0.02
99935432,2.4626417345,-0.0158739847\B,0,-0.7814036516,1.235615009,-0.0
140460175\N,0,-0.7897951431,3.7144261382,0.0084866756\O,0,-1.919720875
3,3.6408667454,0.4293073883\O,0,-0.2098857641,4.6939885135,-0.39547727
69\N,0,3.5557542729,1.3321738663,0.0028024863\O,0,4.0651215347,2.34885
5563,-0.4049972999\O,0,4.1066189932,0.3391053854,0.4148154966\N,0,-0.6
792326001,-1.2411038308,-0.0362506882\O,0,-1.8080549938,-1.2178931916,
-0.4657350393\O,0,-0.059339901,-2.1938968085,0.3723313555\H,0,2.070176
9883,-0.9955154306,-0.0190191514\H,0,1.9679692859,3.5914133937,0.01253
56586\H,0,-1.9529313853,1.2095139363,-0.018576858\\Version=EM64L-G09Re
vA.02\State=1-A\MP2/GTBas1=-853.7621728\CCSD(T)/GTBas1=-853.8621947\MP
2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-851.7406559\MP2/GTMP2LargeX
P=-854.6890891\HF/GFHFB3=-851.7531654\HF/GFHFB4=-851.8122179\G4MP2=-85
5.1474891\FreqCoord=0.0450779388,0.0817574819,-0.0118913542,2.76299813
02,0.0110531905,0.022572324,3.953783398,2.4558635274,-0.0056118587,2.6
556224306,4.8452742029,-0.0434357392,-0.0566795825,4.6537184416,-0.029
9974837,-1.4766389007,2.3349739727,-0.0265431263,-1.4924965216,7.01924
8142,0.0160374926,-3.6277467058,6.8802410352,0.8112733907,-0.396626613
4,8.8703527615,-0.747343745,6.7194017716,2.5174437688,0.0052959317,7.6
819663974,4.4386937397,-0.7653339814,7.7603852293,0.6408163085,0.78388
76843,-1.2835635948,-2.3453463426,-0.0685038729,-3.4167287714,-2.30148
45911,-0.8801116748,-0.1121361616,-4.1458641319,0.7036042926,3.9120675
546,-1.8812515249,-0.0359409874,3.7189229883,6.786787744,0.0236889616,
-3.6905054745,2.2856500936,-0.035105174\PG=C01 [X(B3H3N6O6)]\NImag=0\\
```

methyl-B-trinitroborazine

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.129741 E(Thermal)=                   0.145165
 E(CCSD(T))=              -893.228035 E(Empiric)=                  -0.397824
 DE(MP2)=                   -0.991890 DE(HF)=                      -0.087924
 G4MP2(0 K)=              -894.575933 G4MP2 Energy=              -894.560508
 G4MP2 Enthalpy=          -894.559564 G4MP2 Free Energy=         -894.621439
 1\1\GINC-CL1N064\Mixed\G4MP2\G4MP2\C1H5B3N6O6\KFOREST\14-Jan-2011\0\\#
  G4MP2\\<< job name >>\\0,1\B,0,-0.0005122271,0.001396885,0.0095099129
 \N,0,1.4132474963,0.0342843536,0.0348926904\B,0,2.0847509719,1.2683988
 99,0.0120413315\N,0,1.3473195741,2.4643997535,-0.0177078128\B,0,-0.068
 3211144,2.4248132834,0.001844316\N,0,-0.780111387,1.1918941997,0.01388
 0399\C,0,-2.2633657293,1.1481653569,0.0057068448\N,0,-0.7882116462,3.7
 839792175,0.0054692421\O,0,-1.5540124716,4.0427060916,0.931658446\O,0,
 -0.5140961167,4.5498901735,-0.9151707898\N,0,3.6254512659,1.3133640302
 ,0.0174025092\O,0,4.1612553587,2.4193263022,-0.0273564719\O,0,4.225335
 6906,0.2413889877,0.0659326419\N,0,-0.6525603617,-1.3930864335,-0.0336
 463737\O,0,-1.5599886909,-1.585427057,-0.8398119902\O,0,-0.1925828155,
 -2.2453313799,0.7236138938\H,0,1.9479755814,-0.8228490796,0.0961336484
 \H,0,1.8466640371,3.3426498513,-0.0762421058\H,0,-2.65496261,2.0749249
 811,0.4192960859\H,0,-2.61824843,0.3173895482,0.6148052105\H,0,-2.6329
 263756,1.0050220356,-1.0113516282\\Version=EM64L-G09RevA.02\State=1-A\
 MP2/GTBas1=-893.1156427\CCSD(T)/GTBas1=-893.2280351\MP2/GTBas2=0.\MP2/
 GTBas3=0.\HF/GTMP2LargeXP=-890.9795148\MP2/GTMP2LargeXP=-894.107533\HF
 /GFHFB3=-890.9882507\HF/GFHFB4=-891.0519233\G4MP2=-894.5759326\FreqCoo
 rd=-0.000967969,0.0026397302,0.0179711308,2.6706507259,0.064788039,0.0
 659376289,3.9396083922,2.3969265463,0.0227548187,2.5460650085,4.657040
 616,-0.0334629167,-0.1291081954,4.5822330291,0.0034852522,-1.474196874
 6,2.2523536169,0.0262301528,-4.277141367,2.1697180797,0.0107843737,-1.
 489504146,7.1506844137,0.0103353697,-2.9366579784,7.6396073488,1.76057
 93123,-0.9715008666,8.5980463625,-1.7294221574,6.8511100007,2.48189832
 99,0.0328859765,7.8636329969,4.5718641372,-0.0516962399,7.9847272748,0
 .4561590782,0.1245946365,-1.2331603687,-2.6325518388,-0.0635824317,-2.
 9479513962,-2.9960229415,-1.5870146647,-0.3639287792,-4.2430613855,1.3
 674320853,3.6811403624,-1.5549594091,0.1816662676,3.4896892897,6.31669
 2777,-0.1440766998,-5.017152226,3.9210399605,0.792354771,-4.9477724805
 ,0.5997793236,1.161813473,-4.9755097779,1.8992164049,-1.9111776013\PG=
 C01 [X(C1H5B3N6O6)]\NImag=0\\
```

methyl-N-trinitroborazine

```
Temperature=              298.150000 Pressure=                     1.000000
E(ZPE)=                     0.124602 E(Thermal)=                   0.139450
E(CCSD(T))=              -893.057779 E(Empiric)=                  -0.397824
DE(MP2)=                   -0.984242 DE(HF)=                      -0.089390
G4MP2(0 K)=              -894.404633 G4MP2 Energy=              -894.389785
G4MP2 Enthalpy=          -894.388840 G4MP2 Free Energy=         -894.448587
1\1\GINC-CL1N031\Mixed\G4MP2\G4MP2\C1H5B3N6O6\KFOREST\14-Jan-2011\0\\#
 G4MP2\\<< job name >>\\0,1\N,0,0.0307728769,0.050687604,0.0226378525\
B,0,1.464888195,0.0079953817,0.023809382\N,0,2.1156656375,1.2896393907
,-0.0099047355\B,0,1.41616361,2.5455813325,-0.0065462053\N,0,-0.011985
8616,2.4471820272,0.0606898914\B,0,-0.8162676272,1.2360428126,0.047215
6455\C,0,-2.3777954158,1.1997333754,0.0263678777\N,0,-0.6895576016,3.7
370511447,0.1486987356\O,0,-1.4652929205,3.8705258594,1.0679351015\O,0
,-0.3918252291,4.5459023173,-0.6983673065\N,0,3.5733265186,1.317612436
4,-0.0488707134\O,0,4.0770894773,2.3713507898,-0.3599955449\O,0,4.1342
509589,0.2851250036,0.2334928158\N,0,-0.6094410946,-1.2581727944,-0.01
24319453\O,0,-1.5302480882,-1.3842672633,-0.7879133134\O,0,-0.14969891
66,-2.0902577867,0.7343054006\H,0,2.0496493427,-1.0087980277,-0.013766
8065\H,0,1.9590958072,3.5868699014,0.0058846052\H,0,-2.8363188917,2.14
81502013,0.300134672\H,0,-2.7715155356,0.4263845411,0.6933687969\H,0,-
2.7191552418,0.920961753,-0.976844206\\Version=EM64L-G09RevA.02\State=
1-A\MP2/GTBas1=-892.941958\CCSD(T)/GTBas1=-893.0577789\MP2/GTBas2=0.\M
P2/GTBas3=0.\HF/GTMP2LargeXP=-890.7995585\MP2/GTMP2LargeXP=-893.9262\H
F/GFHFB3=-890.8111745\HF/GFHFB4=-890.87371\G4MP2=-894.4046328\FreqCoor
d=0.0581523097,0.0957856899,0.0427793414,2.7682375039,0.0151090818,0.0
449932114,3.9980286436,2.4370652585,-0.0187172375,2.6761613823,4.81045
15673,-0.0123705352,-0.0226499958,4.6245038288,0.1146872737,-1.5425222
666,2.3357824044,0.0892246393,-4.4933821359,2.267167512,0.0498280676,-
1.3030750198,7.0620032081,0.2809998866,-2.7690023241,7.3142338644,2.01
81048695,-0.740442375,8.5905104065,-1.3197229494,6.7526085036,2.489926
6542,-0.0923522642,7.7045825313,4.4812035577,-0.6802929888,7.812602077
,0.5388081704,0.4412374758,-1.1516767629,-2.3776020092,-0.0234929718,-
2.891749802,-2.6158860224,-1.4889403787,-0.2828899547,-3.9500147641,1.
387636105,3.8732759262,-1.9063519957,-0.026015494,3.7021545437,6.77820
1788,0.0111202922,-5.3598659309,4.0594155727,0.5671723331,-5.237405335
3,0.80575001,1.3102771353,-5.1384587198,1.740365492,-1.8459680239\PG=C
01 [X(C1H5B3N6O6)]\NImag=0\\
```

BH_3

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.025986 E(Thermal)=                   0.028874
 E(CCSD(T))=               -26.484613 E(Empiric)=                  -0.028416
 DE(MP2)=                   -0.044883 DE(HF)=                      -0.003243
 G4MP2(0 K)=               -26.535169 G4MP2 Energy=                -26.532281
 G4MP2 Enthalpy=           -26.531337 G4MP2 Free Energy=           -26.553757
 1\1\GINC-CL1N043\Mixed\G4MP2\G4MP2\B1H3\KFOREST\14-Jan-2011\0\\# G4MP2
 \\name\\0,1\B,0,-1.9258097537,1.22882,0.\H,0,-0.7342180822,1.22882,0.\
 H,0,-2.521611082,2.2607664275,0.\H,0,-2.521611082,0.1968735725,0.\\Ver
 sion=EM64L-G09RevA.02\State=1-A1\MP2/GTBas1=-26.4642438\CCSD(T)/GTBas1
 =-26.484613\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-26.3993502\MP
 2/GTMP2LargeXP=-26.509127\HF/GFHFB3=-26.3995721\HF/GFHFB4=-26.4020012\
 G4MP2=-26.5351692\FreqCoord=-3.6392530186,2.3221332666,0.,-1.387471097
 1,2.3221332667,0.,-4.7651543587,4.2722293984,0.,-4.7651543586,0.372037
 1348,0.\PG=C02V [C2(B1H1),SGV(H2)]\NImag=0\\
```

$B(OH)_3$

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.048360 E(Thermal)=                   0.052777
 E(CCSD(T))=              -251.819258 E(Empiric)=                  -0.113664
 DE(MP2)=                   -0.327823 DE(HF)=                      -0.027454
 G4MP2(0 K)=              -252.239839 G4MP2 Energy=              -252.235423
 G4MP2 Enthalpy=          -252.234478 G4MP2 Free Energy=         -252.266280
 1\1\GINC-CL1N098\Mixed\G4MP2\G4MP2\B1H3O3\KFOREST\14-Jan-2011\0\\# G4M
 P2\\name\\0,1\B,0,-1.9053903645,1.2243521347,0.\O,0,-0.5395376303,1.29
 08192455,0.\O,0,-2.6460020145,2.3738829932,0.\O,0,-2.5306263691,0.0081
 944303,0.\H,0,-0.2211458345,2.1970995169,0.\H,0,-3.5899726105,2.196151
 6387,0.\H,0,-1.9046851766,-0.7204199593,0.\\Version=EM64L-G09RevA.02\S
 tate=1-A'\MP2/GTBas1=-251.7891995\CCSD(T)/GTBas1=-251.8192582\MP2/GTBa
 s2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-251.2994086\MP2/GTMP2LargeXP=-252
 .1170227\HF/GFHFB3=-251.3005459\HF/GFHFB4=-251.3217061\G4MP2=-252.2398
 394\FreqCoord=-3.6006659652,2.3136902248,0.,-1.0195783596,2.4392948611
 ,0.,-5.0002191544,4.4859887287,0.,-4.7821907822,0.0154852291,0.,-0.417
 9050627,4.1519163737,0.,-6.7840650585,4.1501251434,0.,-3.5993333531,-1
 .3613964238,0.\PG=CS [SG(B1H3O3)]\NImag=0\\
```

BF_2H

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.017876 E(Thermal)=                   0.021004
 E(CCSD(T))=              -224.695560 E(Empiric)=                  -0.085248
 DE(MP2)=                   -0.271248 DE(HF)=                      -0.028603
 G4MP2(0 K)=              -225.062784 G4MP2 Energy=              -225.059656
 G4MP2 Enthalpy=          -225.058712 G4MP2 Free Energy=         -225.087118
 1\1\GINC-CL1N043\Mixed\G4MP2\G4MP2\B1F2H1\KFOREST\14-Jan-2011\0\\# G4M
 P2\\name\\0,1\B,0,-1.6780393606,2.1446171469,0.\F,0,-0.3683206114,2.16
 15552528,0.\H,0,-2.300268656,3.1564800856,0.\F,0,-2.284171372,0.983467
 5147,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-224.6780946\C
 CSD(T)/GTBas1=-224.6955604\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP
 =-224.3484063\MP2/GTMP2LargeXP=-224.9493431\HF/GFHFB3=-224.3548716\HF/
 GFHFB4=-224.3726715\G4MP2=-225.0627837\FreqCoord=-3.1710348317,4.05273
 90675,0.,-0.6960250847,4.0847474489,0.,-4.3468777919,5.9648829057,0.,-
 4.3164583336,1.8584842633,0.\PG=CS [SG(B1F2H1)]\NImag=0\\
```

BF_3

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.012472 E(Thermal)=                   0.015974
 E(CCSD(T))=              -323.794193 E(Empiric)=                  -0.113664
 DE(MP2)=                   -0.383618 DE(HF)=                      -0.041056
 G4MP2(0 K)=              -324.320058 G4MP2 Energy=              -324.316557
 G4MP2 Enthalpy=          -324.315612 G4MP2 Free Energy=         -324.346199
 1\1\GINC-CL1N039\Mixed\G4MP2\G4MP2\B1F3\KFOREST\14-Jan-2011\0\\# G4MP2
 \\name\\0,1\B,0,-1.9258269355,1.2288302283,0.\F,0,-0.6187596383,1.2961
 298264,0.\F,0,-2.6376352322,2.327130932,0.\F,0,-2.521098194,0.06318901
 33,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-323.7779786\CCS
 D(T)/GTBas1=-323.7941927\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-
 323.3182352\MP2/GTMP2LargeXP=-324.1615965\HF/GFHFB3=-323.3275855\HF/GF
 HFB4=-323.3530788\G4MP2=-324.3200579\FreqCoord=-3.6392854874,2.3221525
 954,0.,-1.1692862584,2.4493304045,0.,-4.9844082274,4.3976401368,0.,-4.
 7641851408,0.1194099298,0.\PG=CS [SG(B1F3)]\NImag=0\\
```

$BClF_2$

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.010746 E(Thermal)=                   0.014552
 E(CCSD(T))=              -683.785660 E(Empiric)=                  -0.113664
 DE(MP2)=                   -0.359289 DE(HF)=                      -0.039297
 G4MP2(0 K)=              -684.287163 G4MP2 Energy=              -684.283357
 G4MP2 Enthalpy=          -684.282413 G4MP2 Free Energy=         -684.314388
 1\1\GINC-CL1N131\Mixed\G4MP2\G4MP2\B1Cl1F2\KFOREST\14-Jan-2011\0\\# G4
 MP2\\name\\0,1\B,0,-2.0356824927,1.2231398375,0.\Cl,0,-0.2818987002,1.
 3135109784,0.\F,0,-2.7508508296,2.3155169614,0.\F,0,-2.6348979776,0.06
 31322226,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-683.75757
 21\CCSD(T)/GTBas1=-683.7856596\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar
 geXP=-683.330737\MP2/GTMP2LargeXP=-684.1168607\HF/GFHFB3=-683.3441007\
 HF/GFHFB4=-683.3649531\G4MP2=-684.287163\FreqCoord=-3.8468824047,2.311
 3993152,0.,-0.5327113406,2.4821760218,0.,-5.1983547003,4.3756929131,0.
 ,-4.9792355657,0.1193026109,0.\PG=CS [SG(B1Cl1F2)]\NImag=0\\
```

BCl_2H

```
Temperature=              298.150000 Pressure=                     1.000000
E(ZPE)=                     0.014602 E(Thermal)=                   0.018154
E(CCSD(T))=              -944.684595 E(Empiric)=                  -0.085248
DE(MP2)=                   -0.221392 DE(HF)=                      -0.024640
G4MP2(0 K)=              -945.001274 G4MP2 Energy=              -944.997722
G4MP2 Enthalpy=          -944.996778 G4MP2 Free Energy=         -945.027902
1\1\GINC-CL1N072\Mixed\G4MP2\G4MP2\B1Cl2H1\KFOREST\14-Jan-2011\0\\# G4
MP2\\name\\0,1\B,0,-1.7993843573,2.2242024352,0.\Cl,0,-0.0511879353,2.
2340921003,0.\H,0,-2.3904019718,3.2492286637,0.\Cl,0,-2.6837757355,0.7
161768008,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-944.6428
429\CCSD(T)/GTBas1=-944.6845955\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
rgeXP=-944.3782444\MP2/GTMP2LargeXP=-944.8642351\HF/GFHFB3=-944.392439
1\HF/GFHFB4=-944.4008383\G4MP2=-945.001274\FreqCoord=-3.4003436431,4.2
031334667,0.,-0.0967311791,4.2218222252,0.,-4.5172050742,6.1401523175,
0.,-5.0716011422,1.3533780162,0.\PG=CS [SG(B1Cl2H1)]\NImag=0\\
```

BCl_2F

```
Temperature=               298.150000 Pressure=                     1.000000
E(ZPE)=                      0.009075 E(Thermal)=                   0.013184
E(CCSD(T))=              -1043.778814 E(Empiric)=                  -0.113664
DE(MP2)=                    -0.334895 DE(HF)=                      -0.037372
G4MP2(0 K)=              -1044.255670 G4MP2 Energy=              -1044.251561
G4MP2 Enthalpy=          -1044.250617 G4MP2 Free Energy=         -1044.283931
1\1\GINC-CL1N007\Mixed\G4MP2\G4MP2\B1Cl2F1\KFOREST\14-Jan-2011\0\\# G4
MP2\\name\\0,1\B,0,-1.8937366157,1.255879381,0.\F,0,-0.5920091885,1.30
07049698,0.\Cl,0,-2.8110777383,2.7508309154,0.\Cl,0,-2.7060664574,-0.2
986352662,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-1043.738
978\CCSD(T)/GTBas1=-1043.7788137\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2L
argeXP=-1043.3434405\MP2/GTMP2LargeXP=-1044.0738729\HF/GFHFB3=-1043.36
07575\HF/GFHFB4=-1043.3768833\G4MP2=-1044.2556697\FreqCoord=-3.5786435
715,2.3732680861,0.,-1.1187352345,2.4579761725,0.,-5.3121670637,5.1983
17068,0.,-5.1137245019,-0.5643388668,0.\PG=CS [SG(B1Cl2F1)]\NImag=0\\
```

BCl_3

```
Temperature=              298.150000 Pressure=                     1.000000
E(ZPE)=                     0.007410 E(Thermal)=                   0.011842
E(CCSD(T))=             -1403.775094 E(Empiric)=                  -0.113664
DE(MP2)=                   -0.310123 DE(HF)=                      -0.035323
G4MP2(0 K)=             -1404.226795 G4MP2 Energy=             -1404.222363
G4MP2 Enthalpy=         -1404.221418 G4MP2 Free Energy=        -1404.256057
1\1\GINC-CL1N012\Mixed\G4MP2\G4MP2\B1Cl3\KFOREST\14-Jan-2011\0\\# G4MP
2\\name\\0,1\B,0,-2.0006207784,1.2521761062,0.\Cl,0,-0.2515238439,1.32
52282241,0.\Cl,0,-2.9384208867,2.7303905647,0.\Cl,0,-2.812004491,-0.29
9014895,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-1403.72378
29\CCSD(T)/GTBas1=-1403.7750942\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
rgeXP=-1403.3574146\MP2/GTMP2LargeXP=-1404.033906\HF/GFHFB3=-1403.3786
335\HF/GFHFB4=-1403.3899744\G4MP2=-1404.2267947\FreqCoord=-3.780625366
9,2.3662699109,0.,-0.4753111808,2.5043184072,0.,-5.5528107391,5.159690
403,0.,-5.3139183725,-0.5650562613,0.\PG=CS [SG(B1Cl3)]\NImag=0\\
```

$BBrF_2$

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.010177 E(Thermal)=                   0.014172
 E(CCSD(T))=             -2796.521419 E(Empiric)=                  -0.113664
 DE(MP2)=                   -0.686370 DE(HF)=                       -0.093272
 G4MP2(0 K)=             -2797.404548 G4MP2 Energy=             -2797.400552
 G4MP2 Enthalpy=         -2797.399608 G4MP2 Free Energy=        -2797.432948
 1\1\GINC-CL1N086\Mixed\G4MP2\G4MP2\B1Br1F2\KFOREST\14-Jan-2011\0\\# G4
 MP2\\name\\0,1\B,0,-1.920445969,1.1221191928,0.\F,0,-0.6169409091,1.15
 81322469,0.\Br,0,-2.9283082114,2.75534482,0.\F,0,-2.5371949104,-0.0268
 162597,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-2796.505696
 5\CCSD(T)/GTBas1=-2796.5214188\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar
 geXP=-2796.2104944\MP2/GTMP2LargeXP=-2797.1920668\HF/GFHFB3=-2796.2784
 86\HF/GFHFB4=-2796.2988129\G4MP2=-2797.4045479\FreqCoord=-3.6291169345
 ,2.1204979628,0.,-1.1658493584,2.1885527723,0.,-5.5337005522,5.2068471
 116,0.,-4.7946035265,-0.0506753868,0.\PG=CS [SG(B1Br1F2)]\NImag=0\\
```

$BBrCl_2$

```
Temperature=              298.150000 Pressure=                     1.000000
E(ZPE)=                     0.006885 E(Thermal)=                   0.011514
E(CCSD(T))=             -3516.511418 E(Empiric)=                  -0.113664
DE(MP2)=                   -0.637560 DE(HF)=                      -0.089268
G4MP2(0 K)=             -3517.345024 G4MP2 Energy=             -3517.340395
G4MP2 Enthalpy=         -3517.339451 G4MP2 Free Energy=        -3517.375406
1\1\GINC-CL1N100\Mixed\G4MP2\G4MP2\B1Br1Cl2\KFOREST\14-Jan-2011\0\\# G
4MP2\\name\\0,1\B,0,-2.0524508275,1.2018403342,0.\Cl,0,-0.3039757677,1
.1989299964,0.\Br,0,-3.0064393021,2.8604853885,0.\Cl,0,-2.9291441027,-
0.3109657191,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-3516.
4727663\CCSD(T)/GTBas1=-3516.511418\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM
P2LargeXP=-3516.2375766\MP2/GTMP2LargeXP=-3517.110326\HF/GFHFB3=-3516.
3134373\HF/GFHFB4=-3516.3242174\G4MP2=-3517.3450241\FreqCoord=-3.87856
99652,2.271149087,0.,-0.5744309519,2.2656493458,0.,-5.6813469161,5.405
5339914,0.,-5.5352801579,-0.5876400459,0.\PG=CS [SG(B1Br1Cl2)]\NImag=0
\\
```

BBr_2H

```
 Temperature=               298.150000 Pressure=                     1.000000
 E(ZPE)=                      0.013578 E(Thermal)=                   0.017410
 E(CCSD(T))=              -5170.158320 E(Empiric)=                  -0.085248
 DE(MP2)=                    -0.875071 DE(HF)=                      -0.132538
 G4MP2(0 K)=              -5171.237600 G4MP2 Energy=             -5171.233768
 G4MP2 Enthalpy=          -5171.232824 G4MP2 Free Energy=        -5171.266574
 1\1\GINC-CL1N064\Mixed\G4MP2\G4MP2\B1Br2H1\KFOREST\14-Jan-2011\0\\# G4
 MP2\\name\\0,1\B,0,-1.8155256698,2.2521990094,0.\Br,0,0.0887686465,2.2
 78309657,0.\H,0,-2.4058372186,3.2759986541,0.\Br,0,-2.7921557581,0.617
 2026794,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-5170.14166
 02\CCSD(T)/GTBas1=-5170.1583205\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
 rgeXP=-5170.139475\MP2/GTMP2LargeXP=-5171.0167316\HF/GFHFB3=-5170.2629
 543\HF/GFHFB4=-5170.2702383\G4MP2=-5171.2376001\FreqCoord=-3.430846303
 2,4.2560393246,0.,0.1677484311,4.3053812977,0.,-4.5463734634,6.1907402
 679,0.,-5.2764097032,1.1663440326,0.\PG=CS [SG(B1Br2H1)]\NImag=0\\
```

BBr_2F

```
 Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.007969 E(Thermal)=                   0.012478
 E(CCSD(T))=             -5269.250848 E(Empiric)=                  -0.113664
 DE(MP2)=                   -0.989468 DE(HF)=                       -0.145215
 G4MP2(0 K)=             -5270.491225 G4MP2 Energy=             -5270.486717
 G4MP2 Enthalpy=         -5270.485773 G4MP2 Free Energy=        -5270.521120
 1\1\GINC-CL1N106\Mixed\G4MP2\G4MP2\B1Br2F1\KFOREST\14-Jan-2011\0\\# G4
 MP2\\name\\0,1\B,0,-1.9308824466,1.23757,0.\F,0,-0.6312342985,1.23757,
 0.\Br,0,-2.8649466274,2.9095993246,0.\Br,0,-2.8649466274,-0.4344593246
 ,0.\\Version=EM64L-G09RevA.02\State=1-A1\MP2/GTBas1=-5269.2360655\CCSD
 (T)/GTBas1=-5269.2508481\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-
 5269.1033036\MP2/GTMP2LargeXP=-5270.2255336\HF/GFHFB3=-5269.2298224\HF
 /GFHFB4=-5269.2448552\G4MP2=-5270.4912255\FreqCoord=-3.6488390189,2.33
 86683703,0.,-1.1928599499,2.3386683703,0.,-5.4139645112,5.4983458799,0
 .,-5.4139645112,-0.8210091394,0.\PG=C02V [C2(B1F1),SGV(Br2)]\NImag=0\\
```

BBr_2Cl

```
Temperature=               298.150000 Pressure=                     1.000000
E(ZPE)=                      0.006353 E(Thermal)=                   0.011192
E(CCSD(T))=              -5629.248083 E(Empiric)=                  -0.113664
DE(MP2)=                    -0.964943 DE(HF)=                      -0.143127
G4MP2(0 K)=              -5630.463464 G4MP2 Energy=              -5630.458624
G4MP2 Enthalpy=          -5630.457680 G4MP2 Free Energy=         -5630.494950
1\1\GINC-CL1N047\Mixed\G4MP2\G4MP2\B1Br2Cl1\KFOREST\14-Jan-2011\0\\# G
4MP2\\name\\0,1\B,0,-2.0729160075,1.2375724879,0.\Cl,0,-0.3268669874,1
.2375710117,0.\Br,0,-3.0276470789,2.8934598577,0.\Br,0,-3.0276499262,-
0.4183133574,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-5629.
2221832\CCSD(T)/GTBas1=-5629.2480832\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GT
MP2LargeXP=-5629.1178795\MP2/GTMP2LargeXP=-5630.187126\HF/GFHFB3=-5629
.2482932\HF/GFHFB4=-5629.2585153\G4MP2=-5630.4634638\FreqCoord=-3.9172
435507,2.3386730718,0.,-0.617689088,2.3386702821,0.,-5.7214238062,5.46
78467076,0.,-5.7214291867,-0.7904976831,0.\PG=CS [SG(B1Br2Cl1)]\NImag=
0\\
```

BBr_3

```
Temperature=               298.150000 Pressure=                     1.000000
E(ZPE)=                      0.005794 E(Thermal)=                   0.010864
E(CCSD(T))=              -7741.985059 E(Empiric)=                  -0.113664
DE(MP2)=                    -1.292258 DE(HF)=                      -0.196929
G4MP2(0 K)=              -7743.582116 G4MP2 Energy=              -7743.577046
G4MP2 Enthalpy=          -7743.576102 G4MP2 Free Energy=         -7743.614043
1\1\GINC-CL1N124\Mixed\G4MP2\G4MP2\B1Br3\KFOREST\14-Jan-2011\0\\# G4MP
2\\name\\0,1\B,0,-2.1141252119,1.23757,0.\Br,0,-0.2049750422,1.23757,0
.\Br,0,-3.0679898729,2.8911084965,0.\Br,0,-3.0679898729,-0.4159684965,
0.\\Version=EM64L-G09RevA.02\State=1-A1\MP2/GTBas1=-7741.9720137\CCSD(
T)/GTBas1=-7741.9850585\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-7
741.9982921\MP2/GTMP2LargeXP=-7743.2642718\HF/GFHFB3=-7742.1831985\HF/
GFHFB4=-7742.1928653\G4MP2=-7743.5821158\FreqCoord=-3.9951176612,2.338
6683703,0.,-0.3873466939,2.3386683703,0.,-5.7976606383,5.4634032788,0.
,-5.7976606383,-0.7860665382,0.\PG=C02V [C2(B1Br1),SGV(Br2)]\NImag=0\\
```

borazine

```
Temperature=               298.150000 Pressure=                     1.000000
E(ZPE)=                      0.092286 E(Thermal)=                   0.097536
E(CCSD(T))=               -241.923604 E(Empiric)=                  -0.142080
DE(MP2)=                    -0.290829 DE(HF)=                      -0.023101
G4MP2(0 K)=               -242.287328 G4MP2 Energy=              -242.282077
G4MP2 Enthalpy=           -242.281133 G4MP2 Free Energy=         -242.315470
1\1\GINC-CL1N024\Mixed\G4MP2\G4MP2\B3H6N3\KFOREST\14-Jan-2011\0\\# G4M
P2\\name\\0,1\N,0,-0.4631944337,1.2163337345,0.0002256112\B,0,-1.88997
62597,1.2549524804,0.0002253517\N,0,-2.5700784007,0.000001588,-0.00001
18708\B,0,-1.8899798129,-1.2549510626,-0.0002306516\N,0,-0.4631982064,
-1.216334908,-0.0001935599\B,0,0.28371542,-0.0000016815,0.0000255028\H
,0,0.0407943267,2.0889838059,0.0003795829\H,0,-2.4867527303,2.28837898
58,0.0003872202\H,0,-3.5777670354,0.000002833,-0.0000255028\H,0,-2.486
7587457,-2.2883760928,-0.0004091203\H,0,0.040788434,-2.088986204,-0.00
03338844\H,0,1.477297444,-0.0000034786,0.0000413211\\Version=EM64L-G09
RevA.02\State=1-A\MP2/GTBas1=-241.8552048\CCSD(T)/GTBas1=-241.9236043\
MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-241.2415672\MP2/GTMP2Larg
eXP=-242.1460334\HF/GFHFB3=-241.2407779\HF/GFHFB4=-241.2599874\G4MP2=-
242.2873283\FreqCoord=-0.875310626,2.2985376443,0.0004263434,-3.571537
5284,2.3715164978,0.0004258529,-4.8567443173,0.0000030009,-0.000022432
5,-3.571544243,-2.3715138186,-0.0004358684,-0.8753177553,-2.298539862,
-0.0003657753,0.5361444435,-0.0000031776,0.0000481933,0.0770901052,3.9
476072892,0.0007173078,-4.6992816205,4.3244095713,0.0007317402,-6.7609
998641,0.0000053535,-0.0000481934,-4.6992929878,-4.3244041044,-0.00077
31254,0.0770789696,-3.9476118209,-0.00063095,2.791687586,-0.0000065735
,0.0000780855\PG=C01 [X(B3H6N3)]\NImag=0\\
```

G4 archive entries

borazine

```
 Temperature=              298.150000 Pressure=                    1.000000
 E(ZPE)=                     0.092286 E(Thermal)=                  0.097536
 E(CCSD(T))=              -241.923604 E(Empiric)=                 -0.104205
 DE(Plus)=                  -0.019388 DE(2DF)=                    -0.200690
 E(Delta-G3XP)=             -0.345289 DE(HF)=                     -0.022326
 G4(0 K)=                 -242.523216 G4 Energy=                -242.517965
 G4 Enthalpy=             -242.517021 G4 Free Energy=           -242.551357
 1\1\GINC-CL1N148\Mixed\G4\G4\B3H6N3\KFOREST\16-Jan-2011\0\\# G4\\name\
 \0,1\N,0,-0.4631944337,1.2163337345,0.0002256112\B,0,-1.8899762597,1.2
 549524804,0.0002253517\N,0,-2.5700784007,0.000001588,-0.0000118708\B,0
 ,-1.8899798129,-1.2549510626,-0.0002306516\N,0,-0.4631982064,-1.216334
 908,-0.0001935599\B,0,0.28371542,-0.0000016815,0.0000255028\H,0,0.0407
 943267,2.0889838059,0.0003795829\H,0,-2.4867527303,2.2883789858,0.0003
 872202\H,0,-3.5777670354,0.000002833,-0.0000255028\H,0,-2.4867587457,-
 2.2883760928,-0.0004091203\H,0,0.040788434,-2.088986204,-0.0003338844\
 H,0,1.477297444,-0.0000034786,0.0000413211\\Version=EM64L-G09RevA.02\S
 tate=1-A\MP2/GTBas1=-241.8552048\MP4/GTBas1=-241.9211773\CCSD(T)/G3Bas
 1=-241.9236043\MP2/GTBas2=-241.8742444\MP4/GTBas2=-241.940565\MP2/GTBa
 s3=-242.0433869\MP4/GTBas3=-242.1218668\HF/GTLargeXP=-241.2420796\MP2/
 GTLargeXP=-242.4077153\HF/GFHFB1=-241.2599874\HF/GFHFB2=-241.2635402\G
 4=-242.5232162\FreqCoord=-0.875310626,2.2985376443,0.0004263434,-3.571
 5375284,2.3715164978,0.0004258529,-4.8567443173,0.0000030009,-0.000022
 4325,-3.571544243,-2.3715138186,-0.0004358684,-0.8753177553,-2.2985398
 62,-0.0003657753,0.5361444435,-0.0000031776,0.0000481933,0.0770901052,
 3.9476072892,0.0007173078,-4.6992816205,4.3244095713,0.0007317402,-6.7
 609998641,0.0000053535,-0.0000481934,-4.6992929878,-4.3244041044,-0.00
 07731254,0.0770789696,-3.9476118209,-0.00063095,2.791687586,-0.0000065
 735,0.0000780855\PG=C01 [X(B3H6N3)]\NImag=0\\
```

B-nitroborazine

```
Temperature=               298.150000 Pressure=                     1.000000
E(ZPE)=                      0.096001 E(Thermal)=                   0.103860
E(CCSD(T))=               -445.974395 E(Empiric)=                  -0.159781
DE(Plus)=                   -0.036003 DE(2DF)=                     -0.326746
E(Delta-G3XP)=              -0.568463 DE(HF)=                      -0.043265
G4(0 K)=                  -447.012650 G4 Energy=                 -447.004792
G4 Enthalpy=              -447.003847 G4 Free Energy=            -447.045544
1\1\GINC-CL1N073\Mixed\G4\G4\B3H5N4O2\KFOREST\22-Dec-2010\0\\# G4\\<<
job name >>\\0,1\N,0,0.0113433319,0.0302577328,0.006848763\B,0,1.44325
20063,-0.0110126525,0.0069467441\N,0,2.1153101929,1.249068196,-0.00004
15824\B,0,1.4522643535,2.5139153977,-0.0070097126\N,0,0.020097983,2.48
28722509,-0.0068518246\B,0,-0.6677116206,1.2590037326,0.0000177342\N,0
,-2.2196828504,1.2645435522,0.0000382404\O,0,-2.7988372159,0.178777146
7,0.0053763151\O,0,-2.7910764832,2.3544104104,-0.0054075497\H,0,-0.541
415808,-0.8147139026,0.0116792976\H,0,2.037296974,-1.0421599241,0.0127
617606\H,0,3.1237069145,1.2454730917,-0.0000576524\H,0,2.0536611876,3.
5407925956,-0.0128403017\H,0,-0.5266089655,3.3317723725,-0.0116602315\
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-445.8965049\MP4/GTBas1
=-445.9820497\CCSD(T)/G3Bas1=-445.9743945\MP2/GTBas2=-445.93082\MP4/GT
Bas2=-446.0180525\MP2/GTBas3=-446.2030073\MP4/GTBas3=-446.3087952\HF/G
TLargeXP=-444.8191576\MP2/GTLargeXP=-446.8057852\HF/GFHFB1=-444.853888
6\HF/GFHFB2=-444.8607507\G4=-447.0126504\FreqCoord=0.0214357907,0.0571
788284,0.0129422863,2.7273510326,-0.0208108972,0.0131274438,3.99735695
07,2.3603968118,-0.0000785794,2.7443819006,4.7506116229,-0.0132464372,
0.0379796836,4.6919485771,-0.0129480719,-1.2617920987,2.379172255,0.00
00335129,-4.194592689,2.3896409968,0.0000722638,-5.2890358287,0.337839
8461,0.0101597631,-5.2743701692,4.44919088,-0.010218788,-1.0231276011,
-1.5395861525,0.0220706738,3.8499333321,-1.9693968432,0.0241162325,5.9
029505878,2.3536030492,-0.0001089473,3.8808572143,6.691128299,-0.02426
46536,-0.9951467239,6.2961373211,-0.0220346441\PG=C01 [X(B3H5N4O2)]\NI
mag=0\\
```

N-nitroborazine


```
Temperature=              298.150000 Pressure=                     1.000000
E(ZPE)=                     0.094219 E(Thermal)=                   0.101956
E(CCSD(T))=              -445.908411 E(Empiric)=                  -0.159781
DE(Plus)=                  -0.032473 DE(2DF)=                     -0.326392
E(Delta-G3XP)=             -0.567559 DE(HF)=                      -0.043874
G4(0 K)=                 -446.944271 G4 Energy=                 -446.936535
G4 Enthalpy=             -446.935591 G4 Free Energy=            -446.977064
1\1\GINC-CL1N044\Mixed\G4\G4\B3H5N4O2\KFOREST\22-Dec-2010\0\\# G4\\<<
job name >>\\0,1\B,0,-0.0087536656,0.0039299173,-0.0206536001\N,0,1.40
93078005,0.0304874524,-0.0206739195\B,0,2.1940981847,1.223040855,-0.00
02568381\N,0,1.4740889309,2.4557885265,0.0200208441\B,0,0.0594661031,2
.55800347,0.0198631018\N,0,-0.6634319636,1.2993663612,-0.000500914\N,0
,-2.0991223384,1.3377307434,-0.0007322779\O,0,-2.6717848715,0.33416990
06,0.3708700507\O,0,-2.6172408617,2.370443732,-0.3725172294\H,0,-0.623
255369,-1.0036920301,-0.0685833427\H,0,1.8876826236,-0.8567946516,-0.0
505399827\H,0,3.3840840596,1.1912532219,-0.0002220938\H,0,1.9991403421
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END OF SUPPLEMENTARY MATERIAL